



Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 12:57 am BST

PDB ID : 4L5T
Title : Crystal structure of the tetrameric p202 HIN2
Authors : Yin, Q.; Tian, Y.; Wu, H.
Deposited on : 2013-06-11
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

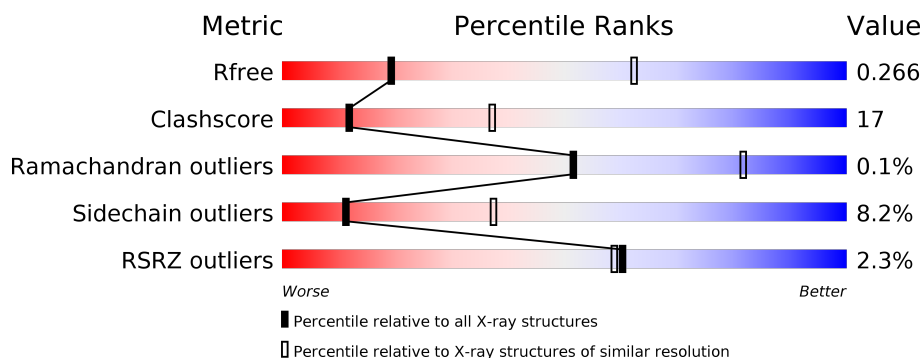
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	203	<div> <div>2%</div> <div> <div></div> <div>62%</div> <div>24%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	203	<div> <div>%</div> <div> <div></div> <div>65%</div> <div>25%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	203	<div> <div></div> <div> <div>56%</div> <div>31%</div> <div>•</div> <div>10%</div> </div> </div>
1	D	203	<div> <div>5%</div> <div> <div></div> <div>58%</div> <div>28%</div> <div>5%</div> <div>10%</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5748 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Interferon-activable protein 202.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	0
			1414	905	229	271	9			
1	B	185	Total	C	N	O	S	0	0	0
			1463	935	240	277	11			
1	C	182	Total	C	N	O	S	0	0	0
			1438	919	236	272	11			
1	D	183	Total	C	N	O	S	0	0	0
			1433	913	237	272	11			

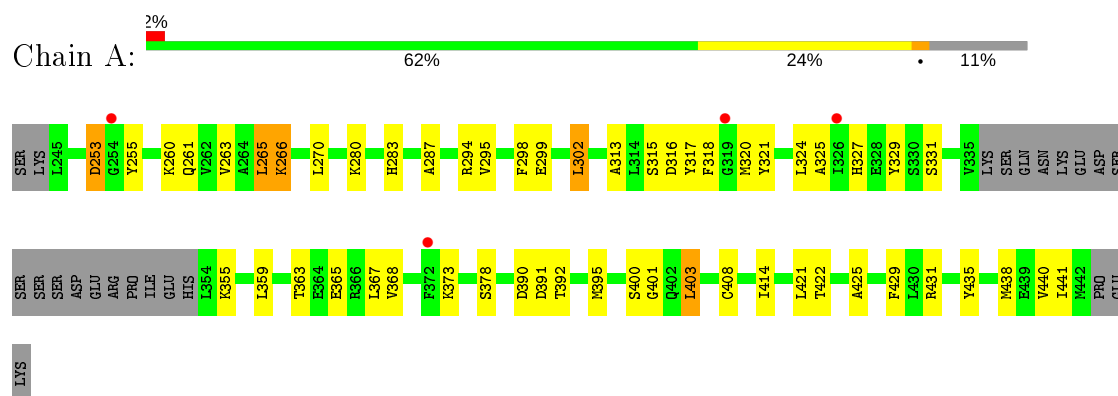
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	243	SER	-	EXPRESSION TAG	UNP Q9R002
A	350	PRO	LEU	VARIANT	UNP Q9R002
A	364	GLU	LYS	VARIANT	UNP Q9R002
A	379	SER	THR	VARIANT	UNP Q9R002
A	432	ALA	SER	VARIANT	UNP Q9R002
B	243	SER	-	EXPRESSION TAG	UNP Q9R002
B	350	PRO	LEU	VARIANT	UNP Q9R002
B	364	GLU	LYS	VARIANT	UNP Q9R002
B	379	SER	THR	VARIANT	UNP Q9R002
B	432	ALA	SER	VARIANT	UNP Q9R002
C	243	SER	-	EXPRESSION TAG	UNP Q9R002
C	350	PRO	LEU	VARIANT	UNP Q9R002
C	364	GLU	LYS	VARIANT	UNP Q9R002
C	379	SER	THR	VARIANT	UNP Q9R002
C	432	ALA	SER	VARIANT	UNP Q9R002
D	243	SER	-	EXPRESSION TAG	UNP Q9R002
D	350	PRO	LEU	VARIANT	UNP Q9R002
D	364	GLU	LYS	VARIANT	UNP Q9R002
D	379	SER	THR	VARIANT	UNP Q9R002
D	432	ALA	SER	VARIANT	UNP Q9R002

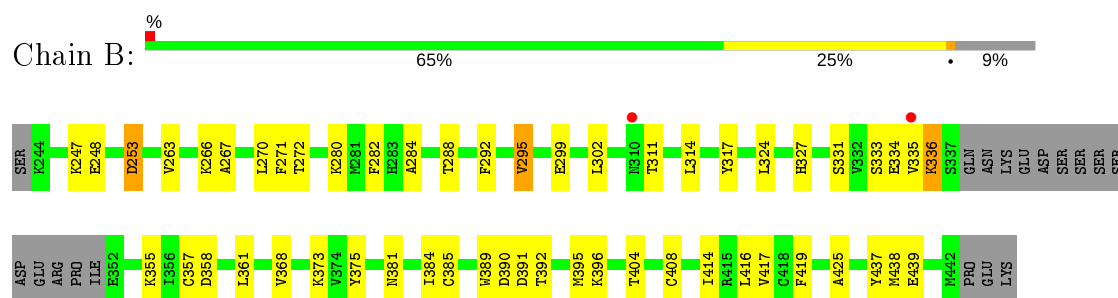
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

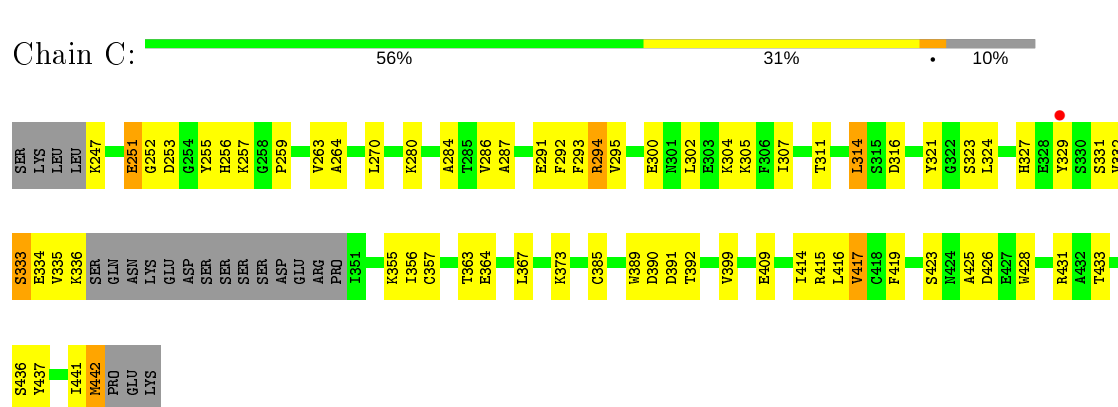
- Molecule 1: Interferon-activable protein 202



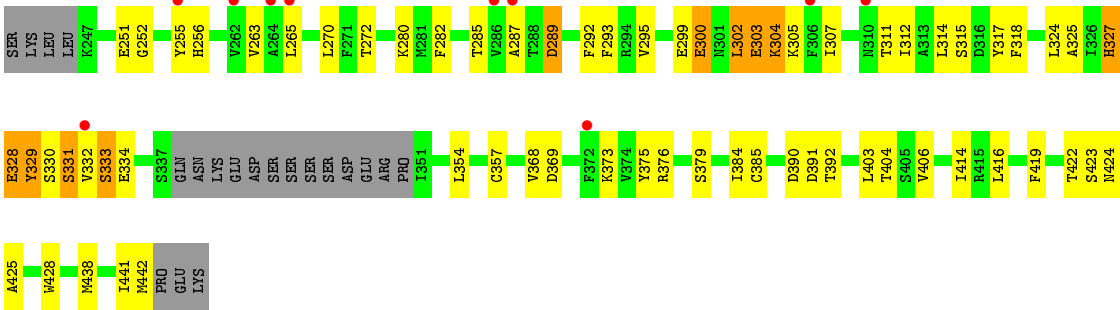
- Molecule 1: Interferon-activable protein 202



- Molecule 1: Interferon-activable protein 202



- Molecule 1: Interferon-activable protein 202



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.89Å 71.86Å 95.47Å 90.00° 102.38° 90.00°	Depositor
Resolution (Å)	46.39 – 3.40 46.39 – 3.41	Depositor EDS
% Data completeness (in resolution range)	97.9 (46.39-3.40) 94.0 (46.39-3.41)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.206 , 0.268 0.208 , 0.266	Depositor DCC
R_{free} test set	1114 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å ²)	80.4	Xtriage
Anisotropy	0.615	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 75.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5748	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.39	0/1441	0.58	0/1943
1	B	0.41	0/1491	0.60	0/2007
1	C	0.40	0/1466	0.60	0/1975
1	D	0.38	0/1460	0.58	1/1966 (0.1%)
All	All	0.40	0/5858	0.59	1/7891 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	304	LYS	C-N-CA	6.26	137.34	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	329	TYR	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1414	0	1375	47	0
1	B	1463	0	1436	32	0
1	C	1438	0	1402	41	0
1	D	1433	0	1392	91	0
All	All	5748	0	5605	196	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (196) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:SER:N	1:D:331:SER:OG	1.58	1.35
1:D:302:LEU:HD11	1:D:328:GLU:O	1.33	1.26
1:D:282:PHE:CE1	1:D:303:GLU:CB	2.23	1.21
1:D:302:LEU:CD1	1:D:328:GLU:O	1.91	1.18
1:A:255:TYR:HB2	1:D:327:HIS:ND1	1.68	1.08
1:D:282:PHE:CE1	1:D:303:GLU:HB2	1.87	1.07
1:A:265:LEU:O	1:A:266:LYS:NZ	1.88	1.06
1:A:365:GLU:N	1:A:365:GLU:OE1	1.91	1.03
1:D:282:PHE:CZ	1:D:303:GLU:HA	1.94	1.00
1:D:302:LEU:HD22	1:D:332:VAL:HG21	1.45	0.99
1:D:270:LEU:HD11	1:D:300:GLU:HB3	1.46	0.97
1:D:299:GLU:OE1	1:D:300:GLU:N	1.99	0.96
1:D:282:PHE:CE1	1:D:303:GLU:HB3	1.99	0.95
1:D:315:SER:CA	1:D:331:SER:OG	2.16	0.94
1:B:357:CYS:HG	1:B:392:THR:HG1	1.10	0.92
1:D:302:LEU:CD2	1:D:332:VAL:CG2	2.48	0.91
1:D:302:LEU:HD22	1:D:332:VAL:CG2	2.01	0.89
1:D:302:LEU:CD2	1:D:332:VAL:HB	2.03	0.89
1:A:255:TYR:HB2	1:D:327:HIS:CE1	2.09	0.88
1:D:328:GLU:HB2	1:D:330:SER:HB2	1.55	0.86
1:A:255:TYR:HD2	1:D:327:HIS:HE1	1.24	0.84
1:A:255:TYR:CD2	1:D:327:HIS:HE1	1.98	0.81
1:D:315:SER:OG	1:D:331:SER:OG	2.00	0.80
1:A:359:LEU:HD23	1:A:421:LEU:HD22	1.64	0.79
1:D:302:LEU:HD21	1:D:332:VAL:HB	1.65	0.79
1:B:295:VAL:HB	1:B:324:LEU:HB2	1.64	0.78
1:D:424:ASN:OD1	1:D:425:ALA:N	2.16	0.78
1:D:302:LEU:CD2	1:D:332:VAL:HG21	2.11	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:357:CYS:H	1:C:392:THR:HG23	1.48	0.76
1:D:327:HIS:C	1:D:328:GLU:HG2	2.06	0.76
1:B:327:HIS:HD2	1:C:255:TYR:HB2	1.48	0.76
1:D:282:PHE:CZ	1:D:303:GLU:CA	2.67	0.76
1:D:302:LEU:CD2	1:D:332:VAL:CB	2.64	0.75
1:B:355:LYS:HB3	1:B:392:THR:HG21	1.68	0.75
1:D:302:LEU:HD11	1:D:328:GLU:C	2.08	0.74
1:A:255:TYR:CD2	1:D:327:HIS:CE1	2.75	0.74
1:D:282:PHE:CE1	1:D:303:GLU:CA	2.71	0.73
1:D:282:PHE:HZ	1:D:303:GLU:HA	1.46	0.73
1:A:265:LEU:HD23	1:A:265:LEU:N	2.03	0.73
1:C:334:GLU:HG3	1:C:335:VAL:N	2.03	0.72
1:D:315:SER:N	1:D:331:SER:CB	2.53	0.71
1:A:265:LEU:HD23	1:A:265:LEU:H	1.57	0.70
1:D:282:PHE:CZ	1:D:303:GLU:HB2	2.27	0.69
1:A:265:LEU:HB2	1:A:266:LYS:HD2	1.75	0.69
1:B:414:ILE:HD12	1:B:416:LEU:HD21	1.76	0.68
1:D:289:ASP:N	1:D:289:ASP:OD1	2.21	0.68
1:D:282:PHE:HE1	1:D:303:GLU:HB3	1.56	0.67
1:D:282:PHE:CD1	1:D:303:GLU:HB2	2.29	0.67
1:D:304:LYS:O	1:D:307:ILE:HG12	1.94	0.67
1:B:253:ASP:OD1	1:B:253:ASP:N	2.27	0.67
1:A:298:PHE:HB2	1:A:327:HIS:HA	1.76	0.66
1:D:302:LEU:CD1	1:D:328:GLU:C	2.64	0.66
1:D:282:PHE:CZ	1:D:303:GLU:CB	2.78	0.65
1:D:327:HIS:O	1:D:328:GLU:HG2	1.96	0.65
1:C:355:LYS:HB3	1:C:392:THR:HG21	1.79	0.64
1:D:299:GLU:OE1	1:D:300:GLU:HG3	1.98	0.64
1:A:265:LEU:C	1:A:266:LYS:HD2	2.18	0.63
1:D:252:GLY:O	1:D:256:HIS:NE2	2.26	0.63
1:D:315:SER:CB	1:D:331:SER:OG	2.46	0.63
1:D:314:LEU:HA	1:D:331:SER:HB3	1.80	0.62
1:D:265:LEU:HD11	1:D:287:ALA:HB2	1.81	0.62
1:A:255:TYR:HD2	1:D:327:HIS:CE1	2.11	0.62
1:B:425:ALA:HB2	1:C:385:CYS:SG	2.40	0.62
1:D:270:LEU:HD11	1:D:300:GLU:CB	2.27	0.61
1:D:327:HIS:H	1:D:327:HIS:CD2	2.16	0.61
1:B:417:VAL:HG22	1:B:437:TYR:HB3	1.82	0.61
1:A:403:LEU:HD13	1:A:438:MET:HB2	1.81	0.61
1:C:255:TYR:HE2	1:C:257:LYS:HB2	1.65	0.61
1:D:272:THR:HG22	1:D:280:LYS:HG2	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:LYS:HB3	1:A:392:THR:HG21	1.82	0.61
1:A:315:SER:O	1:A:331:SER:HB2	2.01	0.60
1:D:302:LEU:HD13	1:D:328:GLU:O	1.94	0.60
1:A:390:ASP:OD1	1:A:391:ASP:N	2.35	0.60
1:B:385:CYS:SG	1:C:425:ALA:HB2	2.42	0.60
1:D:295:VAL:HG12	1:D:324:LEU:HB2	1.84	0.60
1:D:318:PHE:HB3	1:D:325:ALA:HB3	1.84	0.59
1:D:302:LEU:HD23	1:D:332:VAL:HB	1.80	0.59
1:D:270:LEU:HA	1:D:282:PHE:HB3	1.83	0.59
1:A:320:MET:HG2	1:A:321:TYR:HD2	1.68	0.58
1:B:270:LEU:HD21	1:B:280:LYS:HB3	1.85	0.58
1:B:358:ASP:HA	1:B:361:LEU:HD12	1.86	0.58
1:C:251:GLU:HG2	1:C:293:PHE:HE2	1.69	0.58
1:C:270:LEU:HD21	1:C:280:LYS:HB3	1.85	0.57
1:A:403:LEU:HB3	1:A:438:MET:HE3	1.87	0.56
1:C:334:GLU:HG3	1:C:335:VAL:H	1.71	0.56
1:C:294:ARG:HH22	1:C:367:LEU:HB2	1.71	0.56
1:D:414:ILE:HD12	1:D:416:LEU:HD21	1.86	0.55
1:D:282:PHE:CD1	1:D:303:GLU:CB	2.87	0.55
1:A:425:ALA:HB2	1:D:385:CYS:SG	2.46	0.55
1:A:408:CYS:SG	1:A:414:ILE:HD11	2.47	0.54
1:A:265:LEU:HD21	1:A:287:ALA:HB3	1.89	0.54
1:D:251:GLU:HG2	1:D:293:PHE:CE2	2.42	0.54
1:B:390:ASP:OD1	1:B:391:ASP:N	2.41	0.54
1:B:267:ALA:HA	1:B:284:ALA:HA	1.89	0.54
1:D:270:LEU:HD21	1:D:280:LYS:HB3	1.90	0.54
1:D:328:GLU:CB	1:D:330:SER:HB2	2.31	0.54
1:D:384:ILE:HG12	1:D:404:THR:HG22	1.90	0.54
1:C:441:ILE:HG22	1:C:442:MET:HG3	1.90	0.53
1:D:403:LEU:HB3	1:D:438:MET:HE3	1.90	0.53
1:B:263:VAL:HG22	1:B:311:THR:HG22	1.90	0.53
1:D:328:GLU:C	1:D:330:SER:HB2	2.29	0.53
1:C:414:ILE:HD12	1:C:416:LEU:HD21	1.90	0.53
1:C:252:GLY:O	1:C:256:HIS:NE2	2.32	0.53
1:C:294:ARG:NH2	1:C:367:LEU:HB2	2.23	0.53
1:A:263:VAL:HG23	1:A:287:ALA:O	2.09	0.53
1:D:357:CYS:H	1:D:392:THR:HG23	1.72	0.53
1:C:390:ASP:OD1	1:C:391:ASP:N	2.42	0.52
1:B:248:GLU:HG3	1:B:292:PHE:CZ	2.45	0.52
1:A:395:MET:HE2	1:A:429:PHE:HA	1.92	0.52
1:B:368:VAL:N	1:B:419:PHE:O	2.41	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:PHE:HB3	1:A:325:ALA:HB3	1.92	0.51
1:A:270:LEU:HD21	1:A:280:LYS:HB3	1.92	0.51
1:D:302:LEU:HD11	1:D:329:TYR:CA	2.41	0.50
1:A:299:GLU:HB3	1:A:302:LEU:HD12	1.94	0.49
1:C:264:ALA:HA	1:C:286:VAL:HG12	1.95	0.49
1:D:270:LEU:HD12	1:D:303:GLU:HG2	1.95	0.49
1:D:406:VAL:HG21	1:D:438:MET:HB3	1.94	0.48
1:C:259:PRO:HA	1:C:314:LEU:O	2.14	0.48
1:C:270:LEU:CD2	1:C:280:LYS:HB3	2.43	0.48
1:C:416:LEU:HD22	1:C:419:PHE:CZ	2.49	0.48
1:A:265:LEU:CD2	1:A:265:LEU:H	2.19	0.48
1:D:265:LEU:HD12	1:D:285:THR:HG22	1.96	0.48
1:A:261:GLN:HA	1:A:313:ALA:HA	1.95	0.47
1:D:263:VAL:HG22	1:D:311:THR:HG22	1.95	0.47
1:D:373:LYS:HB3	1:D:373:LYS:NZ	2.29	0.47
1:A:294:ARG:HH22	1:A:367:LEU:HB3	1.79	0.47
1:A:400:SER:OG	1:A:401:GLY:N	2.47	0.47
1:B:419:PHE:HZ	1:B:438:MET:HE2	1.79	0.47
1:C:332:VAL:HG12	1:C:333:SER:O	2.14	0.47
1:A:295:VAL:HG12	1:A:324:LEU:HD12	1.96	0.47
1:C:305:LYS:NZ	1:C:329:TYR:OH	2.35	0.47
1:C:433:THR:N	1:C:436:SER:OG	2.45	0.47
1:D:368:VAL:N	1:D:419:PHE:O	2.48	0.47
1:D:328:GLU:HB2	1:D:330:SER:CB	2.35	0.47
1:B:271:PHE:CZ	1:B:437:TYR:HB2	2.50	0.47
1:D:251:GLU:OE2	1:D:317:TYR:OH	2.30	0.46
1:D:302:LEU:HD21	1:D:332:VAL:CG2	2.41	0.46
1:A:431:ARG:HD2	1:D:422:THR:HG23	1.97	0.46
1:A:378:SER:HB2	1:B:381:ASN:OD1	2.15	0.46
1:C:423:SER:HA	1:C:428:TRP:CE2	2.50	0.46
1:D:390:ASP:OD2	1:D:392:THR:HG22	2.15	0.46
1:A:283:HIS:NE2	1:A:435:TYR:O	2.44	0.46
1:C:263:VAL:HG22	1:C:311:THR:HG22	1.96	0.46
1:D:369:ASP:HA	1:D:416:LEU:O	2.15	0.46
1:A:327:HIS:CD2	1:D:255:TYR:HB2	2.50	0.46
1:C:295:VAL:HG12	1:C:324:LEU:HB2	1.98	0.46
1:B:416:LEU:HD22	1:B:419:PHE:CZ	2.51	0.46
1:A:265:LEU:HD21	1:A:287:ALA:CB	2.46	0.46
1:B:299:GLU:HB3	1:B:302:LEU:HD12	1.99	0.45
1:D:302:LEU:HD21	1:D:332:VAL:CB	2.34	0.45
1:A:320:MET:HG2	1:A:321:TYR:CD2	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ASP:OD1	1:A:253:ASP:N	2.41	0.45
1:B:384:ILE:HG12	1:B:404:THR:HG22	1.97	0.45
1:D:302:LEU:O	1:D:305:LYS:HB2	2.17	0.45
1:C:284:ALA:O	1:C:295:VAL:HG22	2.16	0.45
1:C:426:ASP:HB3	1:D:425:ALA:HB3	1.99	0.45
1:D:302:LEU:HD11	1:D:329:TYR:HA	1.98	0.44
1:B:373:LYS:HB3	1:B:373:LYS:HE2	1.79	0.44
1:B:335:VAL:HG12	1:B:336:LYS:N	2.31	0.44
1:D:312:ILE:HD12	1:D:332:VAL:HG13	1.98	0.44
1:A:316:ASP:HB2	1:A:331:SER:HB3	2.00	0.43
1:A:421:LEU:HD12	1:A:422:THR:N	2.33	0.43
1:C:247:LYS:HA	1:C:291:GLU:HA	1.99	0.43
1:C:287:ALA:HA	1:C:292:PHE:HA	2.01	0.43
1:B:375:TYR:HD2	1:B:389:TRP:HB2	1.83	0.43
1:D:331:SER:O	1:D:333:SER:OG	2.33	0.43
1:A:422:THR:OG1	1:A:431:ARG:HG2	2.18	0.43
1:B:271:PHE:CE2	1:B:437:TYR:HB2	2.54	0.43
1:B:395:MET:HG2	1:B:396:LYS:H	1.82	0.43
1:B:270:LEU:HA	1:B:282:PHE:HB3	2.01	0.43
1:B:416:LEU:HD22	1:B:419:PHE:CE1	2.54	0.43
1:C:442:MET:HB2	1:C:442:MET:HE2	1.90	0.43
1:A:373:LYS:HB3	1:A:373:LYS:HE2	1.70	0.42
1:D:287:ALA:HA	1:D:292:PHE:HA	2.01	0.42
1:A:317:TYR:CD2	1:A:324:LEU:HD22	2.54	0.42
1:C:295:VAL:HG12	1:C:324:LEU:HD12	2.02	0.42
1:C:356:ILE:HG13	1:C:390:ASP:OD2	2.19	0.42
1:A:359:LEU:HD21	1:A:368:VAL:HG11	2.02	0.42
1:B:247:LYS:HE3	1:B:247:LYS:HB2	1.84	0.42
1:D:357:CYS:H	1:D:392:THR:CG2	2.32	0.42
1:C:257:LYS:HG3	1:C:316:ASP:OD1	2.20	0.42
1:B:302:LEU:HD23	1:B:302:LEU:HA	1.90	0.41
1:D:375:TYR:CE1	1:D:376:ARG:HD2	2.55	0.41
1:D:423:SER:HA	1:D:428:TRP:CE2	2.55	0.41
1:C:251:GLU:HG2	1:C:293:PHE:CE2	2.51	0.41
1:C:270:LEU:HD11	1:C:300:GLU:HA	2.02	0.41
1:C:417:VAL:HG22	1:C:437:TYR:HB3	2.01	0.41
1:D:441:ILE:HG22	1:D:442:MET:N	2.36	0.41
1:C:373:LYS:HE2	1:C:373:LYS:HB3	1.78	0.41
1:B:317:TYR:CE2	1:B:324:LEU:HD22	2.56	0.41
1:C:415:ARG:HB2	1:C:441:ILE:HD11	2.03	0.41
1:A:255:TYR:CB	1:D:327:HIS:CE1	2.93	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:390:ASP:OD1	1:D:391:ASP:N	2.54	0.40
1:D:302:LEU:HD23	1:D:332:VAL:CB	2.43	0.40
1:C:357:CYS:HB3	1:C:392:THR:O	2.21	0.40
1:C:304:LYS:O	1:C:307:ILE:HG12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	176/203 (87%)	164 (93%)	12 (7%)	0	100	100
1	B	181/203 (89%)	170 (94%)	11 (6%)	0	100	100
1	C	178/203 (88%)	165 (93%)	12 (7%)	1 (1%)	25	57
1	D	179/203 (88%)	166 (93%)	13 (7%)	0	100	100
All	All	714/812 (88%)	665 (93%)	48 (7%)	1 (0%)	51	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	321	TYR

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	153/182 (84%)	143 (94%)	10 (6%)	17	46
1	B	160/182 (88%)	148 (92%)	12 (8%)	13	41
1	C	156/182 (86%)	138 (88%)	18 (12%)	5	20
1	D	155/182 (85%)	144 (93%)	11 (7%)	14	44
All	All	624/728 (86%)	573 (92%)	51 (8%)	11	37

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	ASP
1	A	260	LYS
1	A	265	LEU
1	A	266	LYS
1	A	302	LEU
1	A	329	TYR
1	A	363	THR
1	A	403	LEU
1	A	440	VAL
1	A	441	ILE
1	B	253	ASP
1	B	266	LYS
1	B	272	THR
1	B	288	THR
1	B	295	VAL
1	B	314	LEU
1	B	331	SER
1	B	333	SER
1	B	334	GLU
1	B	336	LYS
1	B	408	CYS
1	B	439	GLU
1	C	251	GLU
1	C	253	ASP
1	C	294	ARG
1	C	302	LEU
1	C	314	LEU
1	C	323	SER
1	C	327	HIS
1	C	331	SER
1	C	333	SER
1	C	336	LYS
1	C	363	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	364	GLU
1	C	389	TRP
1	C	399	VAL
1	C	409	GLU
1	C	417	VAL
1	C	431	ARG
1	C	442	MET
1	D	289	ASP
1	D	300	GLU
1	D	302	LEU
1	D	303	GLU
1	D	327	HIS
1	D	328	GLU
1	D	331	SER
1	D	333	SER
1	D	334	GLU
1	D	354	LEU
1	D	379	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	327	HIS
1	D	360	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	180/203 (88%)	0.20	4 (2%) 62 60	73, 114, 145, 153	0
1	B	185/203 (91%)	-0.06	2 (1%) 80 79	60, 88, 116, 135	0
1	C	182/203 (89%)	-0.03	1 (0%) 91 90	66, 89, 119, 133	0
1	D	183/203 (90%)	0.32	10 (5%) 25 25	84, 116, 142, 158	0
All	All	730/812 (89%)	0.11	17 (2%) 60 59	60, 99, 141, 158	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	287	ALA	4.3
1	D	264	ALA	4.0
1	D	306	PHE	3.7
1	D	265	LEU	3.7
1	D	255	TYR	3.3
1	A	319	GLY	3.1
1	D	286	VAL	2.9
1	A	254	GLY	2.7
1	A	372	PHE	2.6
1	D	262	VAL	2.6
1	A	326	ILE	2.5
1	B	335	VAL	2.5
1	D	372	PHE	2.3
1	B	310	ASN	2.3
1	D	332	VAL	2.2
1	C	329	TYR	2.1
1	D	310	ASN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.